Alternative Hamiltonian Descriptions and Statistical Mechanics

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Abstract

We argue here that, just as it happens in Classical and Quantum Mechanics, where it has been proven that alternative Hamiltonian descriptions can be compatible with a given set of equations of motion, the same holds true in the realm of Statistical Mechanics, i.e. that alternative Hamiltonian descriptions do lead to the same thermodynamical description of any physical system.

In recent years, the research activity in the field of Theoretical Mechanics has brought to the fore the previously unexpected fact that large classes of (classical) dynamical systems can admit of genuinely inequivalent Lagrangian [1] and Hamiltonian [2] descriptions. By "genuinely" we mean here, e.g., Lagrangians that do not differ merely by a so-called total time derivative. As a standard example of this sort we may quote, e.g., the n-dimensional isotropic harmonic oscillator with, for simplicity, unit mass and frequency for which any Hamiltonian of the form:

$$\mathcal{H}_B = \frac{1}{2} B_{ij} (\delta^{ik} p_k \delta^{jl} p_l + q^i q^j) \tag{1}$$

with B a symmetric and nondegenerate $n \times n$ real matrix with constant entries is an admissible Hamiltonian. Similar examples can be exhibited within the Lagrangian formulation of Classical Dynamics as well as at the quantum level [3]. To the best of our knowledge the last case was first considered by E.P.Wigner[4] back in 1950.

The same dynamical evolution can then be compatible with quite different Lagrangian and Hamiltonian formulations and the latter, useful and powerful as they may be, appear to some extent as "superstructures" that can be used interchangeably to describe one and the same dynamical system.

The situation seems to change rather drastically when one moves to Statistical Mechanics, however. Indeed, in their standard formulation [5], both Classical and Quantum Statistical Mechanics appear to be deeply rooted in the Hamiltonian formalism, and the basic quantity out of which one can deduce all the thermodynamic functions that, at equilibrium at least, are the basic observable and measurable quantities, namely the partition function, appears to require the specification of a Hamiltonian and of a symplectic volume in phase space at the classical level or of a Hamiltonian operator and of an Hermitian scalar product in the Hilbert space at the quantum one.

We will argue in this Note that this not quite the case and that (with some necessary technical limitations) alternative Hamiltonian descriptions all yield the same partition function, and hence the same expression for all the observable quantities that can be associated with a given dynamical system.

The general framework we will begin considering is that of the symplectic formulation of Classical Dynamics [6].We start then with a configuration space $\mathbb{Q}$, assumed to be a finite-dimensional smooth manifold, and with a symplectic form Ω on the cotangent bundle $\mathbb{T}^*\mathbb{Q}$. Given any (smooth) function $H \in \mathcal{F}(\mathbb{Q})$, the pair (Ω, H) will determine uniquely the vector field $\Gamma \in \mathcal{X}(\mathbb{T}^*\mathbb{Q})$ such that:

$$i_\Gamma \Omega = -dH \tag{2}$$

Alternatively, the pair (Ω, Γ) will determine the Hamiltonian H upto an additive constant.

We will stick mostly in what follows to the one-dimensional case and to the case in which H is bounded from below (and we will assume then, with

no loss of generality: $H \geq 0$) and the energy "surfaces" are compact. Hence the orbits are closed lines in the two-dimensional phase space. Under these assumptions, the dynamical system associated with the pair $(H, \Omega = dp \wedge dq)$ will be Liouville-integrable [7] and will be described by a single pair (J, ϕ) of action-angle variables. In terms of the latter: $H = H(J), d\phi/dt = \nu \doteq dH/dJ, \Omega = dJ \wedge d\phi$ and the dynamical vector field Γ will be expressed as: $\Gamma = \nu \partial/\partial\phi$.

It is immediate to see that, in the manifold obtained by excluding from the configuration space the critical points of H, the symplectic form Ω can also be written as:

$$\Omega = dH \wedge \xi \tag{3}$$

where:

$$\xi = d(\frac{\phi}{\nu}) \tag{4}$$

is a closed one-form such that: $i_\Gamma \xi = 1$. Locally at least, then, $\xi = dt$ and this will define for us[1] a "time function" t.

Consider as an example a one-dimensional harmonic oscillator with mass m and proper frequency ω, with the standard Hamiltonian:

$$H = \frac{1}{2}\left\{\frac{p^2}{m} + m\omega^2 q^2\right\} \tag{5}$$

Then, on $\mathbb{R}^2 - \{\mathbf{0}\}$ (the origin being the only critical point of H) and, with the standard symplectic form $\Omega = dp \wedge dq$, the vector field will be:

$$\Gamma = \frac{p}{m}\frac{\partial}{\partial q} - m\omega^2 q \frac{\partial}{\partial p} \tag{6}$$

Then:

$$\Omega = dp \wedge dq = dH \wedge \xi \tag{7}$$

with (locally, of course):

$$\xi = dt = \frac{pdq - qdp}{2H} \tag{8}$$

(again "modulo" a multiple of dH), and the "time function" t will be given by: $t = (1/\omega)\tan^{-1}\{m\omega q/p\}$, which emphasizes its local character.

$\mathbb{R}^2 - \{\mathbf{0}\}$ can be identified with $\mathbb{S}^1 \times \mathbb{R}^+$ parametrized by dH and dt. Notice that, denoting by $\Sigma(E)$ the one-dimensional "surface" of constant energy E:

$$\int_{\Sigma(E)} dt = \frac{2\pi}{\omega} \doteq \tau \tag{9}$$

[1]Note that ξ is not unique. Indeed ξ and $\xi + \alpha dH$, with $\alpha = \alpha(H)$ will be just as good. The new one-form will be again closed and it will lead simply to a shift in the origin of the "time function".

with τ the period which, in this specific case, turns out to be a constant independent of the energy. In more general cases $\tau = \tau(E)$ will be a function of the energy.The associated canonical[2] partition function is easily evaluated, and the well-known result[8] is:

$$\mathcal{Z} = h^{-1} \int\limits_{\mathbb{R}^2} \exp\{-\beta H\}\Omega = h^{-1} \int\limits_0^\infty dE \exp\{-\beta E) \int\limits_{\Sigma(E)} dt = \frac{1}{\beta\hbar\omega} \tag{10}$$

Here $\beta = 1/k_B T$ with T the (absolute) temperature and k_B the Boltzmann constant, while h (and: $\hbar = h/2\pi$) is a numerically undetermined constant with the dimension of an action[3] that one is forced [8] to introduce in the context of classical Statistical Mechanics in order to obtain a dimensionless expression for the partition function, so as to make sense of expressions such as : $\mathcal{F} = -\beta^{-1} \ln \mathcal{Z}$ for the (Helmoltz) free energy. As is also well known, the value of h is fixed unambiguously at that of Planck's constant at the quantum level of Statistical Mechanics.

Alternative Hamiltonian descriptions are obtained [3], for a fixed vector field Γ, i.e. for a given set of equations of motion, by changing together H and the symplectic form Ω on $\mathbb{T}^*\mathbb{Q}$ ($\mathbb{Q} = \mathbb{R}$ in our case) in such a way that Γ be again Hamiltonian w.r.t. the new Hamiltonian and symplectic form. Being one-dimensional (and Hamiltonian, hence conservative) implies for our system that any alternative Hamiltonians must necessarily be functions of the initial one (and of each other, of course).

In order to keep track of the correct dimensions of the various physical quantities involved, let's consider a new Hamiltonian of the form:

$$H_\phi = \phi(H) \doteq \beta_0^{-1} f(\beta_0 H) \tag{11}$$

where β_0 is a "fiducial" quantity, fixed once and for all and having dimension $[energy]^{-1}$, and $f(.)$ is a real function. We will assume $f' > 0$ throughout, and that in order: i) to give a sensible meaning to integrals (see below) over phase space and: ii) not to change the number of critical points. The original Hamiltonian will correspond of course to $f(x) = x$.

It is easy to prove that if Γ is Hamiltonian w.r.t. (H, Ω), then it will be Hamiltonian as well w.r.t. (H_ϕ, Ω_ϕ) (i.e.: $i_\Gamma \Omega_\phi = -dH_\phi$), where Ω_ϕ is defined as:

$$\Omega_\phi = dH_\phi \wedge dt \tag{12}$$

Having redefined (through the new symplectic form) the volume element in phase space, it is natural to redefine the partition function as:

$$\mathcal{Z}_\phi = h^{-1} \int\limits_{\mathbb{R}^2} \exp\{-\beta H_\phi\}\Omega_\phi \tag{13}$$

[2]We will restrict here to the canonical ensemble of (both classical and quantum) Statistical Mechanics.

[3]That can be interpreted as the volume of some elementary cell in phase space.

But then:

$$\mathcal{Z}_\phi = -(h\beta)^{-1} \int d \exp\{-\beta E_\phi\} \int\limits_{\Sigma(E_\phi)} dt \tag{14}$$

For the harmonic oscillator it is immediate to see that, again: $\mathcal{Z}_\phi = 1/\beta\hbar\omega$, i.e. that the partition function is insensible to the form of the Hamiltonian *as long as the equations of motion remain the same.*

As another example, consider the following nonlinear (and noncanonical) change of coordinates for the linear oscillator [9](we set here for simplicity: $m = \omega = 1$):

$$Q = q(1+\phi), \quad P = p(1+\phi) \tag{15}$$

where: $\phi = \phi(H) = f(\beta_0 H)$ (cfr. Eq.(11)) and, in our units: $H = (p^2 + q^2)/2$. A straightforward calculation shows that $\Gamma = p\partial/\partial q - q\partial/\partial dp$, which is Hamiltonian w.r.t. the standard pair $(H, \Omega = dp \wedge dq)$, is also Hamiltonian w.r.t. the pair (H', Ω'), where:

$$\Omega' = dP \wedge dQ, \quad H' = (1+\phi)^2 H \equiv \frac{1}{2}(P^2 + Q^2) \tag{16}$$

Explicitly:

$$\Omega' = F(H) dp \wedge dq \tag{17}$$

with:

$$F(H) = (1+\phi)\{1 + \phi + 2H\phi'\} \equiv \frac{dH'}{dH} \tag{18}$$

By writing the symplectic volumes as: $\Omega = dH \wedge dt$ and: $\Omega' = dH' \wedge dt$ respectively[4] and recasting Eq.(23) in the form:

$$\mathcal{Z} = -\frac{1}{\beta h} \int d \exp(-\beta E) \int\limits_{\Sigma(E)} dt \tag{19}$$

it is immediate to see that:

$$\int \exp(-\beta H') dP \wedge dQ = \int \exp(-\beta H) dp \wedge dq \tag{20}$$

i.e. that the partition function remains the same.

These results can be easily generalized. For a general Hamiltonian[5] $H = H(q,p)$ with compact energy "surfaces" and again endowed with a "time one-form" dt (which we know is granted) we can define again a period (energy-dependent in general) $\tau(E)$ as:

$$\tau(E) = \int\limits_{\Sigma(E)} dt \tag{21}$$

[4]This is possible with the **same** time one-form dt precisely because the dynamics is unchanged.

[5]Again in one degree of freedom.

Let's consider the simple case in which the Hamiltonian has just one critical point. Taking the origin at the critical point and setting to zero the minimum of the energy[6]we can evaluate the partition function as:

$$\mathcal{Z} = \lim_{\substack{E\to\infty \\ \varepsilon\to 0}} \left\{ \int_{S(E)} - \int_{S(\varepsilon)} \right\} \exp(-\beta H) \frac{dH \wedge dt}{h} \tag{22}$$

where $S(E)$ (resp. $S(\varepsilon)$) is the volume in phase space bounded by the constant energy surface $\Sigma(E)$ (resp. $\Sigma(\varepsilon)$). Using then Stokes' theorem:

$$\mathcal{Z} = -\frac{1}{\beta h} \lim_{\substack{E\to\infty \\ \varepsilon\to 0}} \left\{ \int_{\Sigma(E)} \exp(-\beta H) dt - \int_{\Sigma(\varepsilon)} \exp(-\beta H) dt \right\} \tag{23}$$

and eventually:

$$\mathcal{Z} = -\frac{1}{\beta h} \lim_{\substack{E\to\infty \\ \varepsilon\to 0}} \{\exp(-\beta E)\tau(E) - \exp(-\beta\varepsilon)\tau(\varepsilon)\} \tag{24}$$

and the desired result obtains immediately by taking the limits. Generalizations to more than one critical point are easily obtained, and we conclude that ("modulo" an essentially irrelevant multiplicative factor multiplicative factor, see footnote 6) *the partition function depends only on the limiting value of the period "at" the critical points of the Hamiltonian.* As the period is entirely determined by the dynamics, and does not depend on the specific Hamiltonian description of the system, this completes the proof in the more general case as well.

We come now to the analogous problem in the context of Quantum Mechanics [4, 10]. In the spirit of the comments that we are making in this Note, and to avoid mathematical complications arising from questions of domains, convergence and the like, we will have in mind mainly a quantum system on a finite-dimensional Hilbert space (a spin, e.g.). This will allow us nonetheless to highlight to some extent the rôle of the various structures involved.

Let's consider then a complex separable Hilbert space $\mathcal{H}$ and and Hamiltonian $\hat{H}$. The latter should be self-adjoint w.r.t. a given Hermitian structure $<,>$ that, together with a linear structure[7], qualifies $\mathcal{H}$ as a Hilbert space. From now on we will call $<,>$ the "standard" Hermitian structure on $\mathcal{H}$. We will assume the spectrum of $\hat{H}$ to be discrete, and to correspond only to a finite

[6]This can always be done whenever, as we assume here, the Hamiltonian is bounded from below. Indeed, shifting the Hamiltonian by a constant: $H \to H + c$ will change the partition function by the multiplicative constant $\exp(-\beta c)$. This implies that the only thermodynamic quantity that will be affected by the shift will be the internal energy: $U =: -\partial \ln \mathcal{Z}/\partial\beta$, which will be shifted by c, leaving all the other thermodynamic functions unchanged [8], and this is perfectly consistent. We will also assume the energy not to be bounded from above.

[7]We will consider here the linear structure as given once and for all, and concentrate on the role of the Hamiltonian and of the Hermitian structure.

number of levels if necessary. Very loosely speaking (see however Ref.[10] for a more accurate analysis involving also the highlighting of the rôle of Kähler structures in Quantum Mechanics) on going from Classical to Quantum Mechanics we replace the rôle of the pair (Ω, H) with that of the pair $(<,>,\hat{H})$.

Adopting the Dirac notation, we will denote by $|\psi\rangle$ the state *vectors* ("*kets*" in Dirac's terminology) and by $\langle\psi|$ their duals (the "*bras*") w.r.t. the given Hermitian structure. Notice that, as a *"bra"* acts on vectors to give scalars, the *"bras"* should be considered more properly as one-forms. Consistently with this we will denote by ψ_k the component of a given ket ψ on a given $O.N.$ basis $\{|k\rangle\}_1^n$ ($n = \dim \mathcal{H}$, and hence: $\mathcal{H} \approx \mathbf{C}^n$ as a vector space) and by ψ^k the corresponding component of the associated bra, i.e.:

$$\psi_k = \langle k|\psi\rangle\,, \quad \psi^k = \langle\psi|k\rangle \tag{25}$$

Observables will be represented (in the present context) by Hermitian matrices: $A = A^\dagger$, and any one of them will be completely specified by the equivalent assignment of the quadratic functional:

$$f_A(\psi) =: \langle\psi|A|\psi\rangle = \psi^k A_k{}^l \psi_l \tag{26}$$

where: $A_k{}^l = \langle k|A|l\rangle$.

The Schrödinger equation is written as:

$$i\hbar\frac{d}{dt}|\psi\rangle = \hat{H}|\psi\rangle \tag{27}$$

or, setting $\hbar = 1$ (or, equivalently, re-defining the Hamiltonian as $\hat{H}/\hbar$) as:

$$i\frac{d\psi_k}{dt} = H_k{}^l \psi_l \tag{28}$$

All this is elementary and well known.

It is then easy to see [10] that the Schrödinger equation can be rewritten as the pair:

$$\frac{d\psi_k}{dt} = -i\frac{\partial f_H}{\partial \psi_k^*}, \quad \frac{d\psi_k^*}{dt} = i\frac{\partial f_H}{\partial \psi_k} \tag{29}$$

Introducing now real coordinates q_k and p^k out of the complex ones[8], the Schrödinger equation can be rewritten as a classical-like set of Hamiltonian equations [11], i.e. as:

$$\frac{dq_k}{dt} = \frac{\partial f_H}{\partial p^k}, \quad \frac{dp^k}{dt} = -\frac{\partial f_H}{\partial q_k} \tag{30}$$

with f_H playing the role of the (classical-like) Hamiltonian.

The Hamiltonian vector field preserves then the Hermitian structure or, equivalently, it is Hermitian w.r.t. the scalar product $<,>$.

[8] And considering then now $\mathbf{C}^n \approx \mathbf{R}^{2n}$ as a real, $2n$-dimensional vector space

Having cast the Schrödinger equation into the Hamiltonian form (30), it is now clear that alternative quantum descriptions can be given by looking for alternative Hermitian structures invariant under the Hamiltonian flow.

Indeed, a new scalar structure allows us to define a new quadratic function:

$$g_A(\psi) =: \langle\psi|A|\psi\rangle_1 \tag{31}$$

and a new Poisson bracket (via the symplectic structure associated with the imaginary part of the Hermitian structure). In this way we get the same equations of motion in the form:

$$\frac{dq_k}{dt} = \frac{\partial g_H}{\partial p^k}; \quad \frac{dp^k}{dt} = -\frac{\partial g_H}{\partial q_k} \tag{32}$$

In deriving these equations we have assumed that the complex structure has been unchanged.

If we consider now the trace of H, if it exists, or of any bounded operator thereof like $\exp\{-\beta H\}$, we have (assuming discreteness):

$$\mathbb{I} = \sum_n |\psi_n\rangle_1 \ {}_1\langle\psi_n| = \sum_n |\psi_n\rangle\langle\psi_n| \tag{33}$$

and

$$Tr\exp\{-\beta H\} = \sum_n \langle\psi_n|\exp\{-\beta H\}|\psi_n\rangle_1 = \sum_n \langle\psi_n|\exp\{-\beta H\}|\psi_n\rangle \tag{34}$$

which is again what we wanted to prove.

All this is recalled here in order to stress that, with some changes, what has been said at the classical level can be carried over also to the quantum-mechanical context. In other words, changing simultaneously the Hamiltonian and the Hermitian structure in such a way that the description of the dynamics w.r.t. the new pair $(\langle,\rangle\,, \widehat{H})$ be unchanged will lead also to the same statistical-mechanical description in the appropriate ensembles, having in mind that the classical integration over phase space w.r.t. the symplectic measure has to be replaced here by the operation of taking traces, the latter depending on the chosen Hermitian structure.

We will consider now the analogous problem in the Heisenbeerg picture. Again for the sake of simplicity, we will consider here only a simple example related to the quantum one-dimensional harmonic oscillator ($QODHO$)[9].

In terms of the creation and annihilation operators a and $a^\dagger$, with the standard commutation relations:

$$[a, a^\dagger] = 1 \tag{35}$$

[9]This will bring us of course beyond finite-dimensional Hilbert spaces, but in a rather easily controlled context, though.

one constructs a basis in the Fock space as:

$$|n>_1 = \frac{(a^\dagger)^n}{\sqrt{n!}}|0\rangle \tag{36}$$

with $|0\rangle$ the Fock vacuum and the standard scalar product, that we will denote as $\langle .|.\rangle_1$:

$$< n|m >_1 = \delta_{nm} \tag{37}$$

The $QODHO$ is described by the Heisenberg equations of motion:

$$\frac{da}{dt} + ia = 0 \tag{38}$$

together with the parent equation for $a^\dagger$, that are obtained in the usual way from the Hamiltonian: $H = a^\dagger a + \frac{1}{2}$. Traces of linear operators are defined then as:

$$Tr_1\hat{O} = \sum_{n=0}^{\infty} \left\langle n|\hat{O}|n \right\rangle_1 \tag{39}$$

with $\hat{O}$ any trace-class operator, of course.

Now, we perform a "nonlinear change of variables" by defining [10] new operators as:

$$A = f(\widehat{n})a \tag{40}$$

with $f(\widehat{n})$ a positive, monotonically increaasing and nowhere vanishing function of the number operator $\widehat{n} = a^\dagger a$ (e.g.: $f(.) = 1 + \tanh(.)$).

At this point, a little care is required when defining the adjoint of any operator, as this notion depends in a crucial way on the hermitian structure we are using on the Hilbert space of states. With the scalar product $\langle .|.\rangle_1$, with which $a^\dagger$ is the adjoint of a, the adjoint of A is of course: $A^\dagger = a^\dagger f(\hat{n})$

It is pretty clear that $\widehat{n}$ being a constant of the motion the equations of motion for A and $A^\dagger$ will be the same as before. We can however reconstruct a different Fock space by assuming the same vacuum and defining new states[10] as:

$$|n>_2 = \frac{(A^\dagger)^n}{\sqrt{n!}}|0> \tag{41}$$

with a **new** scalar product to be declared as:

$$< n|m >_2 = \delta_{nm} \tag{42}$$

[10]Note that, with this definition: $|n\rangle_2 = \{\prod_{k=0}^{N-1} f(k)\}|n\rangle_1$

The nonlinearity of the transformation reflects itself in the fact that, despite the fact that (see the previous footnote) $|n\rangle_1$and $|n\rangle_2$ are proportional, the linear structure in the Fock space labeled by "1" does not carry over to the linear structure of space "2". This has to do with the fact that the proportionality factors between the $|n\rangle_1$'s and the $|n\rangle_2$'s depend on n. In other words, if we try to induce on space "2" a linear structure modelled on that of space "1", the latter will not be compatible with the bilinearity of the scalar product $\langle .|.\rangle_2$ that we have just defined.

We may also wish to compute the commutator of the operators A and $A^\dagger$. This is easily done and we find:

$$[A, A^\dagger] = \Phi(\hat{n}+1) - \Phi(\hat{n}) \tag{43}$$

where: $\Phi(x) = xf^2(x)$.

Now, $A^\dagger$ is no more the adjoint of A w.r.t. the new Hermitian structure we have introduced. If we denote by $(.)_2^\dagger$ the adjoint of any operator w.r.t. the second Hermitian structure, then we find:

$$(A^\dagger)_2^\dagger = \frac{1}{f(\hat{n})}a \tag{44}$$

which is quite different from A. The pair $\{(A^\dagger)_2^\dagger, A^\dagger\}$ will yield a new ("non-linear") realization of the Heisenberg algebra, and indeed it is immediate to see that:

$$[(A^\dagger)_2^\dagger, A^\dagger] = 1 \tag{45}$$

Now, $(A^\dagger)_2^\dagger$ and $A^\dagger$ will obey the same equations of motion as a and $a^\dagger$, that can be derived from the previous commutation relations and from the Hamiltonian: $\widetilde{H} = A^\dagger(A^\dagger)_2^\dagger + 1/2$ (which turns out actually to coincide with the old one when written in terms of the original creation and annihilation operators) and that will have therefore the same spectrum. Defining then consistently the trace of any operator $\hat{O}$ as:

$$Tr_2\hat{O} = \sum_{n=0}^{\infty} \left\langle n|\hat{O}|n \right\rangle_2 \tag{46}$$

will lead to the same partition function.

The examples discussed here seem therefore to point to the result that, both in the classical as well as in the quantum case, the Hamiltonian description is a sort of "superstructure" that is imposed on the thermodynamic description of physical systems, and that what really matters are the equations of motion of the systems themselves.

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